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Effective Sommerfeld parameters in the three-body Coulomb continuum problem

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The three-body Coulomb continuum wave function as a product of three two-body Coulomb wave functions is modified by the introduction of an *Ansatz* for effective Sommerfeld parameters corresponding to the modification of a particular two-body Coulomb interaction by the presence of the third particle. The triple-differential cross sections for electron-impact ionization of atomic hydrogen at incident energies of 54.4 and 150 eV in asymmetric geometry are calculated. We generally find that this approach gives good agreement with experiment, though some small quantitative discrepancies remain. [S1050-2947(97)50110-7]

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The process of electron-impact ionization of atoms has attracted wide interest both experimentally and theoretically for many years. The experiment determines the incident energy E_0, the final-state electron energies E_1 and E_2, and the corresponding momenta $\mathbf{k}_1$ and $\mathbf{k}_2$. As a result, the kinematics of each ionizing event is fully determined and the most detailed information, i.e., the triple-differential cross section (TDCS) is provided. For theorists, the challenge has been to develop a theory capable of explaining these observations. For energies greater than about six times the ionization energy, several different approaches are in reasonable agreement with the existing data. However, the problem of the low-energy ionization process is still one of the basic unsolved problems of atomic physics, although a number of theoretical studies have been devoted to this problem. Particularly noteworthy are the pseudostate close-coupling (PSCC) calculations of Curran and Walters [1], the three-body distorted-wave Born approximation (3DWBA) calculations of Jones *et al.* [2], the convergent close-coupling (CCC) calculations of Bray *et al.* [3], and the work of Berakdar and Briggs [4].

It is well known that a significant advance in the theory of electron-impact ionization was achieved by Brauner, Briggs, and Klar [5] (hereafter to be referred to as BBK), who performed the first calculation for electron-atom ionization using a final-state wave function that satisfied the asymptotic three-body Schrödinger equation exactly. Unfortunately, the BBK model is not in agreement with the measurements for low energies. As can be seen in Ref. [4], the major limitation of the BBK work lies in the fact that influence on the strength of the interaction of any two particles by the presence of a third one has not been taken into account. So, Berakdar and Briggs corrected the deficiency of the BBK wave function, while still maintaining the philosophy, by the introduction of effective Sommerfeld parameters in the two-body factors in the BBK wave function [4], and the results turned out to be in good agreement with experimental findings over a wide range of collision geometry [4,6]. Note that the modification performed by Berakdar and Briggs [4] is limited for the case in which the escaping electrons have equal energies. Based on the same consideration, Berakdar has successfully derived an approximate analytical solution of the quantum-mechanical three-body Coulomb continum problem [7]. However, this work is not very practical.

The goal of the present paper is to advance the work of Berakdar and Briggs [4] by formulating the effective Sommerfeld parameters for any case to modify the BBK wave function. For convenience, now the BBK wave function is referred to as 3C because it is a product of three Coulomb wave functions. The Sommerfeld parameter $\alpha = Z_a Z_b \mu_a \mu_b / k_{ab}$ is a measure of the strength of the Coulomb interaction between particles of charged Z_a and Z_b, reduced mass μ_{ab}, and relative momentum $k_{ab} = \mu_{ab} |\mathbf{k}_a - \mathbf{k}_b|$ conjugate to $r_{ab} = |\mathbf{r}_a - \mathbf{r}_b|$. Because the strength of the interaction of any two particles is affected by the presence of a third particle, the new Sommerfeld parameters introduced here are functions of all three relative momenta. The modification of the strength of a particular two-body Coulomb interaction depends on the momenta of the two particles relative to the third one in question, which represents a dynamic screening (DS) of the three two-body Coulomb interactions and hence the new wave function will be designated as DS3C. As can be seen in Ref. [4], the new momentum-dependent Sommerfeld parameters β_i are introduced simply by a linear transformation from the original set α_i, i.e.,

$$\beta_i = \sum_{j=1}^{3} A_{ij} \alpha_j , \tag{1}$$

where the nine coefficients $A_{ij} \in \mathbb{R}$ and $i = 1$, 2, or 12 designate the two-body interaction of the two electrons with the residiual ion and the electron-electron interaction, respectively; and the condition

$$\beta_1 + \beta_2 + \beta_{12} = \alpha_1 + \alpha_2 + \alpha_{12} \tag{2}$$

should be satisfied. The original two-body Sommerfeld parameters are

$$\alpha_1 = -\frac{Z}{k_1}, \quad \alpha_2 = -\frac{Z}{k_2}, \quad \alpha_{12} = -\frac{1}{2k_{12}}, \tag{3}$$

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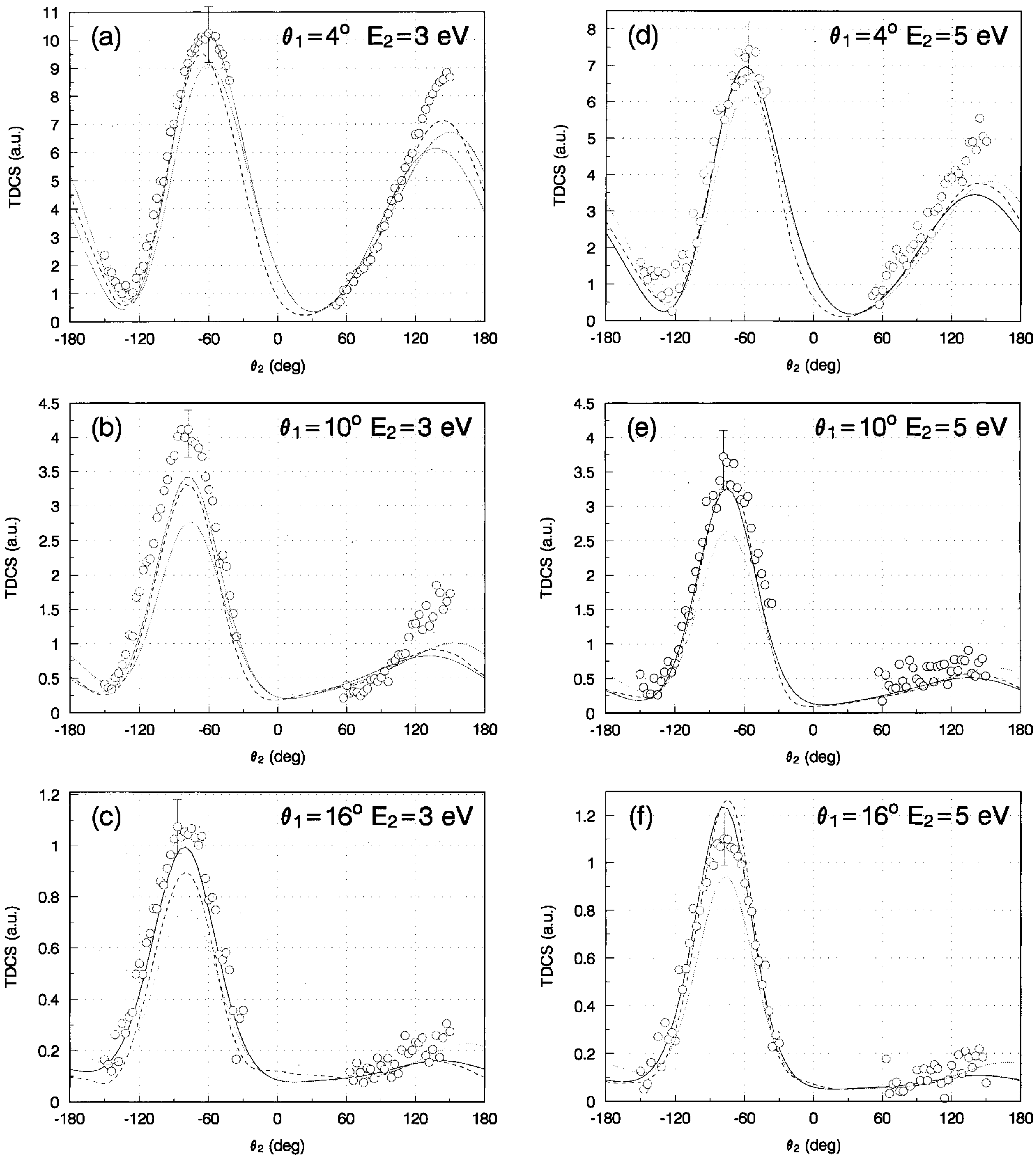

FIG. 1. TDCS for electron-impact ionization of hydrogen at incident energy $E_0=150$ eV. The circles are the experimental measurements of Ehrhard *et al.* [10]. Theories: solid curve, DS3C of this work; broken curve, CCC of Ref. [3]; dotted curve, 3C of Ref. [5].

where Z is the charge of the residiual ion.

For the symmetric case $k_1=k_2=k$, the new Sommerfeld parameters are readily given by Berakdar and Briggs [4], as

$$\beta_1=\beta_2=-\frac{Z-\sin\theta/4}{k}, \tag{4}$$

$$\beta_{12}=\frac{1-\sin^2\theta}{2k\,\sin\theta} \tag{5}$$

where $\theta=(\cos^{-1}\hat{\mathbf{k}}_1\cdot\hat{\mathbf{k}}_2)/2$ varies from $\pi/2$ to zero. It is easy to find that when $\theta=\pi/2$, $\beta_{12}=0$. The classical interpretation is that when the residual ion is between the two elec-

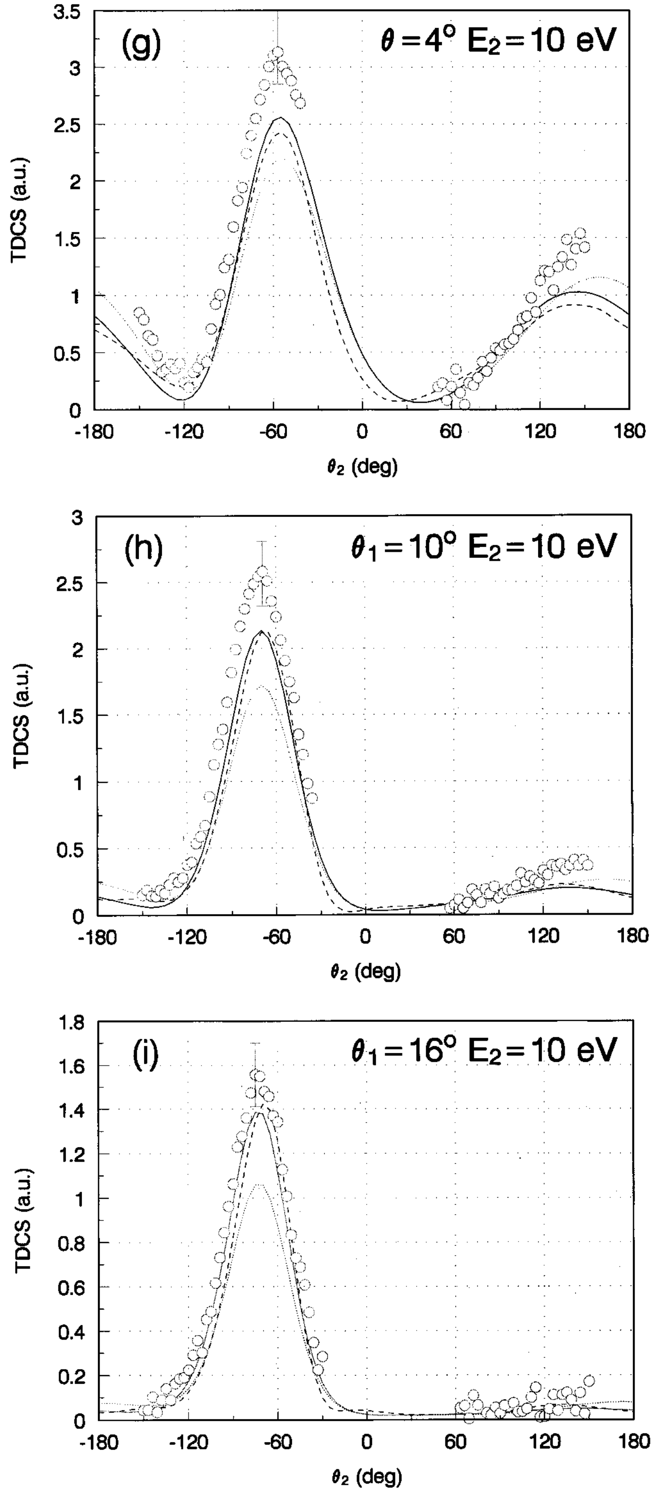

FIG. 1. *(Continued).*

trons the electron-electron interaction is subsumed *completely* in an effective electron-ion interaction. However, this is only true for the symmetric case considered in Ref. [4]. For the asymmetric case $k_1 \neq k_2$, the electron-electron interaction cannot be subsumed completely by the effective electron-ion interaction when $\theta=\pi/2$ and hence $\beta_{12}\neq 0$. On the other hand, for the two outgoing electrons, the effective charge of the ion registered by one electron reduces as the momentum of this one increases due to the screening of the

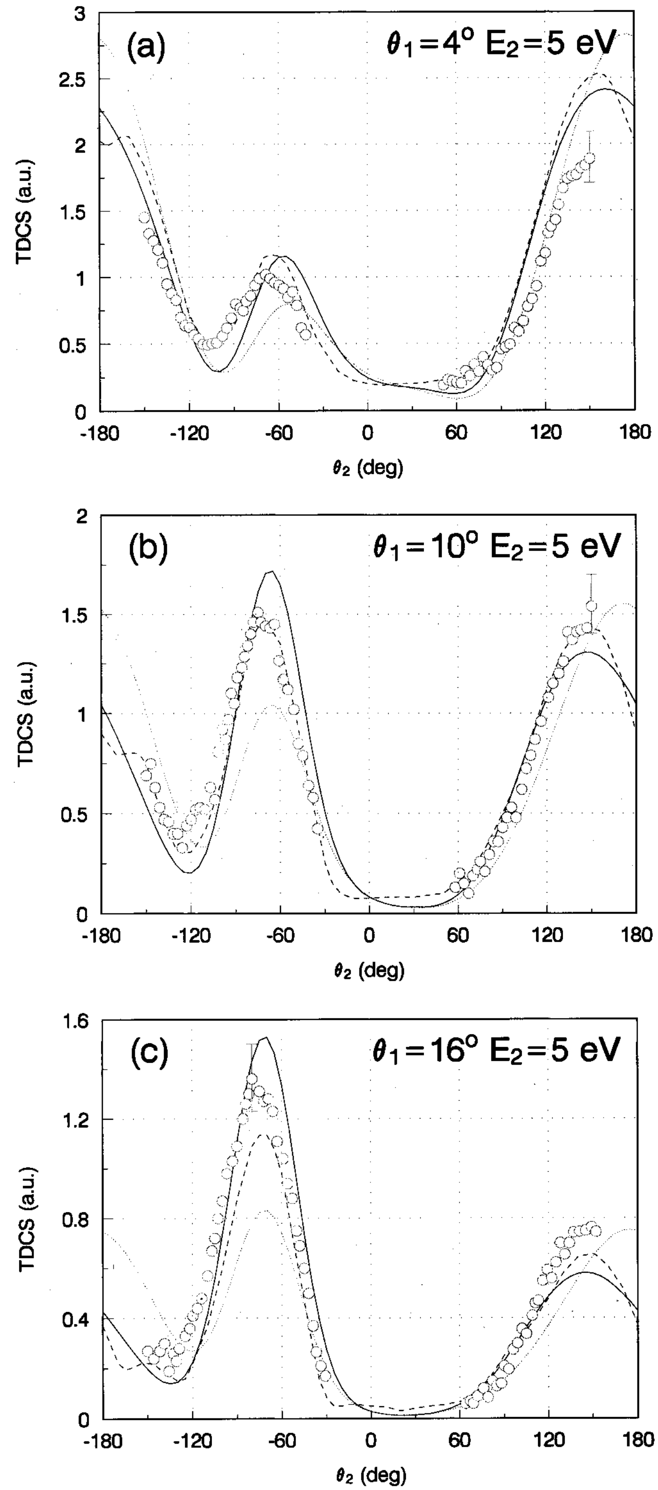

FIG. 2. TDCS for electron-impact ionization of hydrogen at incident energy $E_0=54.4$ eV. The circles are the relative measurements of Brauner *et al.* [11]. Theories; solid curve, DS3C of this work; broken curve, CCC of Ref. [3]; dotted curve, 3C of Ref. [11].

other electron. Then the effective charge of the ion registered by the two outgoing electrons should be in the range $Z-1<Z_{\mathrm{eff}}\leqslant Z$, and $Z^{i}_{\mathrm{eff}}\rightarrow Z$ as $k_j\rightarrow\infty$ $(i\neq j;\ i,j=1,2)$. Based on this consideration, we finally arrive at the representation of the new Sommerfeld parameters for any geommetry case, as

$$\beta_1 = -\frac{Z - \frac{k_1}{4k_{12}}(\sin^2\theta)\left(1 - \frac{|k_1 - k_2|}{4k_{12}}\right)}{k_1}, \qquad (6)$$

$$\beta_2 = -\frac{Z - \frac{k_2}{4k_{12}}(\sin^2\theta)\left(1 - \frac{|k_1 - k_2|}{4k_{12}}\right)}{k_2}, \qquad (7)$$

$$\beta_{12} = \frac{1 - (\sin^2\theta)\left(1 - \frac{|k_1 - k_2|}{4k_{12}}\right)}{2k_{12}}. \qquad (8)$$

Note that when $k_1 = k_2$, the above representation is identical to those of Ref. [4] [Eqs. (4) and (5)].

In an earlier paper [8], we have calculated the TDCS for electron-impact ionization of helium in a symmetric coplanar energy-sharing geometry at incident energies from 45 to 500 eV and an angle of 45° using the DS3C wave function presented by Berakdar and Briggs [4], and found excellent agreement with the absolute measurement [9]. In this work, we apply the present DS3C wave function to the calculatation of TDCS for electron-impact ionization of hydrogen in asymmetric geometry. To our knowledge, the latest lowest-incident-energy measurements available for hydrogen in asymmetric geometry are due to Ehrhardt *et al.* [10] and Brauner *et al.* [11].

In Fig. 1 the present TDCS results for a projectile energy of 150 eV together with the 3C [5] and CCC [3] results are compared with the experiment. The experimental data are relative measurements for three angles of the fast electron and three energies of the slow electron normalized experimentally [10]. It can be seen that the present results are in very good agreement with the CCC results and experiment. The 3C underestimate of cross sections in the binary peak is corrected by the DS3C. However, the DS3C still underestimates the cross section in the recoil peak for small scattering angles of 4° and 10°. The fact that the two significantly different theories are in good agreement with each other but not with the experimental data for these cases is striking and difficult to explain. Further experimental investigation would be very helpful.

In Fig. 2 are shown the 54.4-eV results. The measurements of Brauner *et al.* [11] are not absolute and have been normalized using the best visual fit to CCC theory using a single multiplicative constant [3]. The present DS3C calculations also show the improvement over the 3C results in obtaining better magnitudes and shapes, and continue to be in agreement with the experimental data and the CCC calculations, while neither the PSCC nor the 3DWBA predict the qualitative shape of the experimental data at this energy (the results of PSCC and 3DWBA are not shown in this paper but can be seen in Refs. [3,2]), although both the approaches are in good ageement with experiment at an energy of 150 eV. The location of the binary peak predicted by the 3DWBA is shifted by about 20° from experiment [2]. The 20° shift in the binary peak for 54.4 eV might stem from the fact that the asymptotic form of the final-state electron-electron correlation factor is used in the 3DWBA. Furthermore, although the 3DWBA has used the distorted wave for the initial state, the results of 3DWBA are not in better agreement with experiment than those of the present DS3C. So, it may be deduced that employment of the distorted wave for the initial state is not very helpful for electron-atom collisions, provided that the correct wave function for the final state is used.

Recently, Jones *et al.* [12] have also performed the calculations for electron-impact ionization of hydrogen at 150 and 54.4 eV using the DS3C model proposed by Berakdar [7]. However, their results turned out to be in worse agreement with experiment than the present results.

In summary, a different approach to the three-body Coulomb continuum, in which new Sommerfeld parameters are introduced for both symmetric and asymmetric cases, gives good agreement with the experiment and the CCC calculations and hence shows the improvement over the BBK results in obtaining better magnitudes and shapes of cross sections. This modification of the BBK wave function has removed its major deficiency.

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[1] E. P. Curran and H. R. J. Walters, J. Phys. B **20**, 337 (1987).
[2] S. Jones, D. H. Madison, A. Franz, and P. L. Altick, Phys. Rev. A **48**, R22 (1993).
[3] I. Bray, D. A. Konovalov, I. E. McCarthy, and A. T. Stelbovics, Phys. Rev. A **50**, R2818 (1994).
[4] J. Berakdar and J. S. Briggs, Phys. Rev. Lett. **72**, 3799 (1994).
[5] M. Brauner, J. S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[6] J. Berakdar and J. S. Briggs, J. Phys. B **27**, 4271 (1994).
[7] J. Berakdar, Phys. Rev. A **53**, 2314 (1996).
[8] S. Zhang, Z. Chen, Q. Shi, and K. Xu, Z. Phys. D (unpublished).
[9] A. Pochat *et al.*, Phys. Rev. A **47**, R3483 (1994).
[10] H. Ehrhard, K. Jung, G. Knoth, and P. Schlemmer, Z. Phys. D **1**, 3 (1986).
[11] M. Brauner *et al.*, J. Phys. B **24**, 657 (1991).
[12] S. Jones, D. H. Madison, and D. A. Konovalov, Phys. Rev. A **55**, 444 (1997).